CHANNEL MODELING OF MULTILAYER DIFFUSION-BASED MOLECULAR NANO COMMUNICATION SYSTEM

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To my beloved father, mother, wife and sons for their endless love, encouragement and support.

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ABSTRACT

In nanoscale communication, diffusion-based molecular communication (DBMC) in which information is encoded into molecule patterns by a transmitter nanomachine, has emerged as a promising communication system, particularly for biomedical and healthcare applications. Although, numerous studies have been conducted to evaluate and analyze DBMC systems, investigation on DBMC system through a multilayer channel has received less attention. The aims of this research are to mathematically model a closed-form expression of mean molecular concentration over multilayer DBMC channel, to formulate channel characteristics, and to conduct performance evaluation of multilayer DBMC channel. In the mathematical model, the propagation of molecules over an n-layer channel is assumed to follow the Brownian motion and subjected to Fick's law of diffusion. The partial differential equation (PDE) of the time rate change of molecular concentration is obtained by modeling the n-layer channel as an n-resistor in series and considering the conservation law of molecules. Fourier transform and Laplace transform were used to obtain the solution for the PDE, which represents the mean molecular concentration at a receiver nanomachine. In the formulation, channel characteristics such as impulse response, time delay, attenuation or the maximum peak, delay spread and capacity were analytically obtained from the mean molecular concentration. In this stage, the multilayer channel is considered as a linear and deterministic channel. For the performance evaluation, the air-water-blood plasma medium representing the simplified multilayer diffusion model in the respiratory system was chosen. It was found that both analytical and simulation results of mean molecular concentration using Matlab and N3Sim were in good agreement. In addition, the findings showed that the higher the average diffusion coefficient resulted in a smaller dispersion of channel impulse response, and shortened the channel delay spread as well as time delay. However, the channel attenuation remains unchanged. In the performance evaluation, an increase of 100% in the transmission distance increased the time delay by 300% but decreased the maximum peak of molecular concentration by 87.5%. A high channel capacity can be achieved with wide transmission bandwidth, short transmission distance, and high average transmitted power. These findings can be used as a guide in the development and fabrication of future artificial nanocommunication and nanonetwork systems involving multilayer transmission medium. Implication of this study is that modeling and analyzing of multilayer DBMC channel are important to support biomedical applications as diffusion can occur through a multilayer structure inside the human body.

ABSTRAK

Dalam komunikasi berskala nano, komunikasi berdasarkan peresapan molekul (DBMC) di mana maklumat dikodkan ke dalam pola molekul oleh pemancar mesin nano telah muncul sebagai satu sistem komunikasi berpotensi di masa hadapan, khususnya untuk aplikasi-aplikasi bio-perubatan dan penjagaan kesihatan. Walaupun banyak kajian telah dijalankan untuk menilai dan menganalisis sistem DBMC, namun kajian ke atas sistem DBMC melalui saluran banyak lapisan masih kurang mendapat perhatian. Tujuan kajian ini adalah untuk memodelkan secara matematik ungkapan tertutup bagi penumpuan purata molekul merentasi saluran DBMC banyak lapisan, pemformulaan ciri-ciri bagi saluran dan penilaian prestasi bagi saluran DBMC banyak lapisan. Dalam permodelan matematik, pergerakan molekul merentasi n-lapisan saluran adalah diandaikan mengikuti gerakan Brownian dan tertakluk kepada hukum peresapan Fick. Persamaan pembezaan separa (PDE) bagi penumpuan purata molekul berubah terhadap masa diperoleh dengan memodelkan n-lapisan saluran sebagai n-perintang secara sesiri dan mempertimbangkan hukum keabadian molekul. Jelmaan Fourier dan jelmaan Laplace telah digunakan untuk mendapatkan penyelesaian bagi PDE, yang mewakili penumpuan purata molekul di penerima mesin nano. Dalam pemformulaan, ciri-ciri bagi saluran seperti sambutan impuls, kelewatan masa, perlemahan atau puncak maksimum, kelewatan penyebaran dan kapasiti telah diperoleh secara analisis daripada ungkapan penumpuan purata molekul. Di peringkat ini, saluran banyak lapisan dianggap sebagai satu saluran yang linear dan berketentuan. Untuk penilaian prestasi, saluran udara-air-plasma darah yang mewakili model ringkas peresapan banyak lapisan bagi sistem respirasi telah dipilih. Di dapati bahawa kedua-dua keputusan analisis menggunakan Matlab dan simulasi menggunakan N3Sim bagi penumpuan purata molekul adalah selari. Selain itu, keputusan-keputusan ini juga menunjukkan bahawa semakin tinggi pekali resapan purata, mengakibatkan semakin kecil penyebaran sambutan impuls bagi saluran dan memendekkan kelewatan penyebaran saluran dan juga kelewatan masa.Walau bagaimanapun, pelemahan saluran adalah kekal tidak berubah. Dalam penilaian prestasi saluran DBMC banyak lapisan, penambahan jarak penghantaran sebanyak 100% meningkatkan kelewatan masa sebanyak 300% tetapi mengurangkan penumpuan puncak maksimum molekul sebanyak 87.5%. Kapasiti saluran yang tinggi boleh dicapai dengan lebar jalur penghantaran yang besar, jarak penghantaran yang pendek dan kuasa penghantaran purata yang tinggi. Dapatan kajian ini boleh digunakan sebagai panduan di dalam pembangunan dan pembuatan sistem komunikasi nano dan rangkaian nano tiruan masa depan yang melibatkan saluran penghantaran banyak lapisan. Implikasi kajian ini adalah menerusi permodelan dan penganalisisan saluran DBMC banyak lapisan yang penting bagi menyokong aplikasi-aplikasi bio-perubatan memandangkan peresapan molekul boleh berlaku melalui banyak struktur lapisan di dalam tubuh manusia.

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LIST OF ABBREVIATIONS

BANs	-	Body Area Nanonetworks
dB	-	Decibel
C	-	Celcius
CSK	-	Concentration Shift Keying
DBMC	-	Diffusion-Based Molecular Communication
Hz	-	Hertz
IoBNT	-	Internet of Bio-Nano Things
ISI	-	Inter-Symbol Interference
MoSK	-	Molecule Shift Keying
OOK	-	On-Off Keying
ODE	-	Ordinary Differential Equation
PAM	-	Pulse Amplitude Modulation
PDE	-	Partial Differential Equation
RN	-	Receiver Nanomachine
TN	-	Transmitter Nanomachine
W	-	Watt

LIST OF SYMBOLS

$\delta(r)$	-	Dirac's delta function of the source location
$\delta(t)$	-	Dirac's delta function of the source time
η	-	Dynamic viscosity of the fluidic medium
η_{air}	-	Dynamic viscosity of air
η_{water}	-	Dynamic viscosity of water
η_{blood}	-	Dynamic viscosity of blood plasma
τ_h	-	Channel delay spread
$*$	-	Convolution operation
$v_0 - v_1$	-	Voltage difference
∇^2	-	Laplacian operator
$\frac{\partial}{\partial x}\hat{i}+\frac{\partial}{\partial y}\hat{j}+\frac{\partial}{\partial z}\hat{k}$	-	Three-dimensional gradient operator
$\frac{\partial c(r,t)}{\partial r}$	-	Molecular concentration gradient
$\frac{\partial c(r,t)}{\partial t}$	-	Time rate changes in molecular concentration
$\frac{dc(r,t)}{dt}$	-	First time derivative of mean molecular concentration
ℓ	-	Total thickness of the propagation medium
ℓ/D	-	Diffusive resistance of the medium
ℓ_i/D_i	-	Diffusive resistance of the i-layer
ℓ_i/ℓ	-	Fraction of the i-layer
Δc	-	Cocentration difference of molecules
Δr	-	Membrane thickness
$c(x,y,z,t)$	-	Mean molecular concentration in three dimensional space at time t
$c(r,t)$	-	Mean molecular concentration
$c(r_0,t)$	-	Concentration of molecules at the location of TN

$c(r_0 + \ell, t)$	-	Concentration of molecules at the location of RN
$c(r, t)_{max}$	-	Channel attenuation, or maximum peak of mean molecular concentration
$c_r(r, t)$	-	First space derivative of mean molecular concentration
$c_{rr}(r, t)$	-	Second space derivative of mean molecular concentration
$c_t(r, t)$	-	First time derivative of mean molecular concentration
$c_t(\omega, t)$	-	First time derivative of Laplace transforms of $C(\omega, t)$
$erfc$	-	Complementary error function
f_i	-	Fraction of the i-layer
$f_x(x)$	-	Probability density function of all the possible transmitted signal X
$h(r, f)$	-	Transfer function Fourier transform of the channel impulse response
$h(r, t)$	-	Channel impulse response
i	-	An integer 1, 2, 3, ...
$inverfc$	-	Inverse operation of the complementary error function
k	-	Partition coefficient of membrane
k_B	-	Boltzmann constant
n	-	Number of layers
r	-	Transmission distance or TN-RN distance
r_m	-	Radius of molecules
r_s	-	Radius of receiver sensing volume
$s(r, t)$	-	Mean number of received molecules
t	-	Time
t_d	-	Time delay
A	-	Area
C	-	Channel capacity
D	-	Diffusion coefficient
D_{av}	-	Average diffusion coefficient
D_i	-	Diffusion coefficient of the i-layer
$H(X)$	-	Entropy per second of the transmitted signal X

$H(Y)$	-	Entropy per second of the received signal Y
$H(\hat{Q})$	-	Entropy of the number of transmitted molecules per time sample of the time function signal $Q(t)$
$H(X,Y)$	-	Joint entropy per second of the transmitted signal X and the received signal Y
$H(X\|Y)$	-	Conditional entropy per second of the transmitted signal X given the received signal Y
I	-	Current
$I(X;Y)$	-	Mutual information
J	-	Flux or diffusion rate per unit area
$J(x,t)$	-	Net diffusion flux at x and at time t
$J(x+\ell,t)$	-	Net diffusion flux at $x+\ell$ and at time t
$J(r,t)$	-	Net radial diffusion flux
$\vec{J}(x,y,z,t)$	-	Flux vector in three dimensional space at time t
$N(x,t)$	-	Molecules at position x and time t
$N(x+\delta$,t)	-	Molecules at position $x+\delta$ and time t
dN	-	Net number of particles
P	-	Permeability coefficient
$\bar{P}_{\mathcal{H}}$	-	Average thermodynamic power in molecules transmission
Q	-	Total number of transmitted molecules
Q_0	-	Total number of transmitted molecules
Q_{ave}	-	Average number of transmitted molecules
$Q(t)$	-	Time function of molecule transmission
R	-	Resistance
R_b	-	Data rate of transmitted bits
T	-	Temperature
T_b	-	Pulse bit duration
T_s	-	Symbol duration or interval
V	-	Receiver sensing volume
dV	-	Differential volume
W	-	Bandwidth of the transmitted signal

X	-	Transmitted or input signal
Y	-	Received or output signal
$C(\omega, t)$	-	Fourier transforms of $c(r, t)$
$F(\omega)$	-	Fourier transforms of $\delta(r)$
$\overline{C}(\omega, s)$	-	Laplace transforms of $C(\omega, t)$
$\overline{F}(s)$	-	Laplace transforms of $\delta(t)$

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CHAPTER 1

INTRODUCTION

1.1 Background

Rapid development in nanotechnology has motivated nanocommunication and nanonetworks of large numbers of nanoscale devices or nanomachines. Nanocommunication is a new research area where a communication process occurs between nanomachines. In a nanonetwork, a group of nanomachines is interconnected among them and expected to share information and coordinate activities to perform a specific task. With nanonetworks, the limited capabilities of a single nanomachine, such as only for computation, sensing, or actuation, can be expanded for executing more complex tasks and a wide range of applications. Interaction among networked nanomachines will allow the implementation of collaborative and synchronous tasks such as in-body drug delivery, disease treatments, and monitoring and controlling of environmental pollution [1].

Generally, nanocommunication can be realized through four different mechanisms, which are nanomechanical communication through mechanical contact, acoustic communication by using acoustic energy or pressure variations, nano-electromagnetic communication based on the modulation of terahertz electromagnetic waves, and molecular communication via transmission and reception of encoded information molecules [1]. However, both nano-electromagnetic communication and molecular communication have been envisioned as the two main options for wireless nanocommunication and nanonetworks [2]. Due to a small-scale, bio-compatible with the biological environment and energy efficiency of a molecular transceiver, molecular communication offers the most promising approaches for nanocommunication and nanonetworks among biological nanomachines as well as with the existing biological system [1, 3–6]. Another reason is that molecular communication can be approached through the observation of existing natural phenomena in biology [2, 7].

In the past decade, research activities have shown significant interests in the area of molecular communication to realize nanocommunication and nanonetworks. Numerous research efforts can be found in the literature to investigate the various models of molecular communication. Some of the proposed models are random walk [8,9], flow based or random walk with drift [10–12], diffusion based [2,3,12–15], diffusion-reaction based [16], walkway or active transport based [8, 17, 18] and collision based [19]. The performances of the proposed models are then analyzed in terms of channel capacity [9, 10], modulation schemes [9], normalized gain and delay [3], probability of reaching a receiver [17], transmission rate [11,12,15,17,18], mutual information [10, 11], noise [13], throughput and efficiency [14], signal attenuation and amplification [16], collision rate [19], and communication range [15].

Among the proposed channel models, molecular communication by diffusion or diffusion-based molecular communication (DBMC) with and without drift has been the focus of interest in the research community [20]. The DBMC channel model is chosen as it represents the most basic and widespread molecular communication architecture found in nature [21, 22]. The concept of congestion in the DBMC channel for drug delivery near the targeted or disease area is introduced in [20]. A drug delivery system model using the DBMC with drift for drug transportation over bloodstream to only unhealthy parts inside the body can be found in [23]. Recently, the concept of body area nanonetworks (BANs) with DBMC for healthcare applications has been introduced in [5]. Furthermore, the concept of the Internet of Bio-Nano Things (IoBNT), involving the DBMC model for intra-body communication can be found in [24]. It is expected that from the proposed IoBNT, a healthcare provider can retrieve certain intra-body status parameters, such as glucose, sodium, and cholesterol levels, and the presence of unwanted agent through bio-nano things inside the body by using the Internet connection. The term bio-nano things can be referred to any type of nanosystems including liposomes [25–27], dendrimers [28], metallic nanoparticles [29], polymeric nanoparticles [30], carbon nanotubes [31] and nanowires [32, 33].

The current developments of nanotechnology in nanomedicine, tissue engineering, nanorobots, bio-sensor, bio-marker, and implant technologies have provided the possibilities of an intelligent system for an early disease detection and spontaneous targeted drug delivery in the treatment of human diseases in the near future. In these intelligent systems, a group of bio-nanomachines embedded in the human body or implanted under the skin are expected to communicate and cooperatively share information using molecular signals among each other or with the surrounding cells to perform a specific function such as synthesis the human health

condition, identifying the targeted drug delivery locations, and automatically control the amount and time of drug release. Moreover, the molecules of the drug are expected to be able to diffuse across a multilayer barrier or multiple environments towards the bloodstream as well as to the other parts inside the body or the infected area. Thus, a better understanding of how the drug's molecules diffusing over the body and its concentration over time are utmost important for an effective disease treatment with an optimum amount of drugs.

1.2 Problem Statement

In nanoscale communication, the DBMC has emerged as one of the most promising communication models, particularly for health monitoring and drug delivery applications. In the DBMC, a transmitter nanomachine (TN) translates a message into encoded molecules and transmits them to a propagation medium or channel by opening a molecular gate. The transmitted molecules are then propagated from the TN to a receiver nanomachine (RN) over the channel by a diffusion process via Brownian motion. The RN captures the encoded molecules propagating in the channel and finally decodes the captured molecules.

Although, numerous studies have been conducted to evaluate and analyze DBMC system, investigation on DBMC through a multilayer channel due to variations in the medium properties or medium temperature has had less attention. The propagation of molecules over various mediums and environments or more complex medium, such as intracellular environment and the human body needs to be considered [4]. In practice, the diffusion of molecules can occur over the several layers in the human body, for example, diffusion of oxygen and carbon dioxide over the alveolar-blood barrier in the respiratory system [34], diffusion of digested particles, nutrients or medicine across the stomach-blood barrier during the absorption process, and diffusion of water, oxygen, carbon dioxide and lipid-soluble molecules through the blood-brain barrier [34]. Additionally, a tissue, particularly an arterial wall, which has the different material properties in each layer, is commonly modeled as a multilayer medium [35, 36].

However, no works have been reported throughout the literature that analytically modeled and evaluated the performance of multilayer DBMC channel from the perspective of communications and an information theory. It is still not

clear how molecules will propagate through the multilayer DBMC channel that is consisting of different medium properties or different medium temperature. Thus, it is utmost important to develop a mathematical model to predict the concentration profile over time and characterize how molecules will propagate over a multilayer channel. Modeling and analysis of molecules' propagation over a multilayer channel with different medium properties are important to be explored in order to support the future biomedical applications such as regulating the release of drugs over a multilayer structure of environment in living tissue, as well as for the BANs and IoBNT applications. Therefore, this research work is proposed to model and evaluate the performance of multilayer DBMC channel.

1.3 Research Objectives

The main objective of this research is to mathematically model and evaluate the performance of multilayer DBMC channel. This research study has the following specific objectives:

(i) To develop a mathematical model of multilayer DBMC channel in deriving a closed-form expression of the mean molecular concentration at the RN location.

(ii) To formulate channel characteristics of multilayer DBMC channel.

(iii) To evaluate the performance of the multilayer DBMC channel generated from different medium properties.

1.4 Research Scopes

In order to achieve the objectives, the following scopes have been employed:

(i) The research focuses on mathematical modeling of a point to point (a pair of nanomachines) DBMC channel without any noise sources or propagation impairments to derive the mean molecular concentration at the RN location over a multilayer channel. Furthermore, the propagation of molecules from the point-source TN to the point and passive RN is governed by the Fick's law of diffusion.

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